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Physica E 29 (2005) 154–174
PHYSICA E
www.elsevier.com/locate/physe

Long and short time quantum dynamics: I. Between Green's functions and transport equations

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Available online 18 July 2005

Abstract

This paper summarizes the present views on construction of the electron quantum transport equations based on the Non-Equilibrium Green's Functions approach. The basic tool is the so-called Ansatz decoupling; one Ansatz family stems from the original Kadanoff-Baym Ansatz and is suitable for extending the quasi-particle picture of the Landau theory out of equilibrium. The other family based on the Generalized KB Ansatz is appropriate for short time transients. The physical and formal context of the Ansatzes is analyzed; the most important question explored is the status of the Reconstruction Theorems, reducing a full description of a non-equilibrium system to a dynamic theory in terms of one-particle quantities. A comparison is made between the Time Dependent Density Functional Theory and the properly renormalized NGF formalism. There is a close relationship between both formalisms. The Reconstruction Theorems form a general basis for obtaining improved quantum transport equations.

PACS: 05.30.−d; 05.60.Gg; 72.10.Bg; 73.23.−b; 31.15.Mb; 31.15.Ew

Keywords: Non-equilibrium; Green functions; Quantum transport equations; Density Functional Theory

1. Introduction

This paper is the first one of three contributions to this volume ([1], hereafter called Paper II, [2], hereafter called Paper III) devoted to quantum transport out of equilibrium, that is to say, beyond the linear response. We concentrate on a specific question of generating reliable transport equations for electrons in extended systems driven by external fields under various conditions which might be broadly divided into "slow" and "fast" phenomena, represented by quasi-stationary quantum transport, and optical or transient processes, respectively. We need to describe both regimes properly. As the underlying general description of non-equilibrium systems, we will use the Non-equilibrium Green's Functions (NGF) [3–9] – double-time correlation

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doi:10.1016/j.physe.2005.05.014

functions which include full quantum sub-dynamics of interactions in the presence of arbitrary external fields and/or in highly non-equilibrium transient states. The NGF can be used to describe actual systems directly, but we presently discuss the methods of an approximate reduction of the theory to equations for single-time quantities, quantum distribution functions. The approximations are based on hierarchy of characteristic times of a given system and they all have "Ansatz" in their name with reference to the original, so-called Kadanoff–Baym Ansatz (KBA) [3,8].

In agreement with the above division of phenomena to slow and fast, the basic formalism forks into two specific lines of developing single-time evolution equations. The common "intuitive" tool to describe transport experiments (long time behavior) is a quantum generalization of the Boltzmann equation (BE) [3–12]. It is based on the concept of a quasi-particle distribution function and on the quasi-classical approximation suitable if everything varies smoothly in space and time. In the NGF context, the mild time dependence, in particular, is a necessary condition for the validity of the KBA, which has been devised to obtain the quantum generalizations of the Boltzmann equation. We will call this type of evolution equations the Quantum Kinetic Equations (QKE). Further progress in this direction led to an extension of the Ansatz incorporating off-shell propagation in an effective manner. The resulting modified scheme has been used to obtain the quantum BE with the corresponding corrections [6,13–15].

If a smooth time dependence cannot be assumed, a more complete quantum treatment becomes necessary to describe the short time (transient) and high-frequency processes. For states far from equilibrium, a theory interpolating adequately between the fully quantum linear response (…the standard Kubo formula, whose use is limited to weak external fields acting on an equilibrium system) and the quasi-classical high-field BE is needed. Such a theory may be based on the quantum Generalized Master Equations (GME) [8,9,16,12] with a strictly causal structure. These equations abandon the quasi-particle distribution concept and describe the evolution of the density matrix (or Wigner function) for true particles. The tool for generating the GME within the NGF environment is a correspondingly structured Ansatz usually called Generalized KB Ansatz (GKBA) [17–20,8,9]. Also this Ansatz can be further developed and refined to obtain an improved GME with a wider range of applicability [8,9].

It is remarkable that more than 40 years since the inception of the KBA, and almost 20 years since its modification to the GKBA, this area of non-equilibrium physics is still active and developing, as witnessed by the number of papers and of meetings devoted to it [21–23]. The questions addressed range from the practice of employing the quantum transport equations to the justification, extension and refinement of the Ansatz-based bridge between the NGF and other quantum transport approaches. These problems are the subject matter of the present paper series.

It should be stressed that similar questions and tasks emerge in very small metal and semiconductor systems. Quantum coherence plays an essential role in the behavior of such systems. A natural question emerges to how the behavior of such systems corresponds to the "classical" way of description known from classical thermodynamics and statistical physics. We attempt to describe a unifying approach to non-equilibrium dynamics, which, while based on studies of extended systems, is also well suited for systems with a reduced dimensionality.

Summary of Papers I, II, III

This Paper I and the adjoining Papers II, III are not intended as an exhaustive review. They rather try to stress the basic issues from our point of view. This is especially true of this first one. The subject matter is divided roughly as follows. In this paper, we present an overview of the basic concepts and of the formal means used. The paper culminates in the last section devoted to the *reconstruction problem*: to what extent can the non-equilibrium dynamics of the many-particle system be described in terms of the evolution of the one-particle distribution? Paper II is devoted to the case of the quasi-particle transport in quasi-classical

environment, as described by the QKE. The Kadanoff-Baym Ansatz and its extensions are analyzed in full detail. Finally, Paper III studies the GME approach to strongly non-equilibrium processes. This is connected with the physics, improvements and generalizations of the GKBA. Special attention is paid to the proper treatment of initial conditions, which are crucial for the early evolution of transients.

2. Definitions and symbols

The average values, for all additive (single-particle) observables $A(x,p)$, are given by the single particle reduced density matrix:

$$A_{\mathrm{Av}}(t) = \mathrm{tr}(\rho(t)A)\ , \tag{1}$$

$$\begin{aligned}\rho(x,y,t) &= \mathrm{TR}\big(\hat{\rho}\psi^{\dagger}(y,t)\psi(x,t)\big),\\ &\equiv \langle\!\langle\ \psi^{\dagger}(y,t)\psi(x,t)\ \rangle\!\rangle\ .\end{aligned} \tag{2}$$

Here $\hat{\rho}$ is the full many-body statistical operator (typically, a grand canonical density matrix) and $\psi^{\dagger}$ and ψ are field operators for particles (electrons throughout this article), all in the Heisenberg picture.

In particular, the local particle density n of electrons is given by

$$n(x,t) = \rho(x,x,t)\ . \tag{3}$$

For a single band $\epsilon(k)$, the local current density j equals

$$j(x,t) = \frac{1}{2m}\left(\frac{\partial\epsilon}{\partial k}(i\nabla_x) + \frac{\partial\epsilon}{\partial k}(-i\nabla_y)\right)\rho(x,y,t)\bigg|_{y=x}. \tag{4}$$

A good starting point for the real-time NGF approach is to extend, following Kadanoff and Baym [3], the single-time reduced electron density matrix ρ to a double-time function, the so-called electron correlation function

$$g^{<}(1,2) = \langle\!\langle\ \psi^{\dagger}(2)\psi(1)\ \rangle\!\rangle, \tag{5}$$

where, instead of x, t we introduce cumulative variables denoted by numbers, $1 \equiv x_1, t_1$, $\alpha \equiv x_\alpha, t_\alpha$.

The single-electron reduced density matrix is then the time-diagonal element of this correlation function

$$\rho(x_1,x_2,t) = g^{<}(1,2)\big|_{t_{1,2}=t}. \tag{6}$$

A complete set of correlation functions is obtained by introducing a complementary function, the correlation function for holes

$$g^{>}(1,2) = \langle\!\langle\ \psi(1)\psi^{\dagger}(2)\ \rangle\!\rangle. \tag{7}$$

For these two functions $g^{<}$, $g^{>}$, Kadanoff and Baym developed a closed set of coupled dynamic equations, the KB formalism [3,8]. In parallel, Keldysh created a basically equivalent matrix formulation of the NGF approach [24,25,5]. See Section 7.

Remark on Conventions: This section introduces most of the writing conventions used in this paper. There is no special symbol for single-particle operators, while many-body quantities have a cap. Single-particle trace ...tr, many-particle trace ...TR. Commutator ...[...]_, anti-commutator ...[...]$_+$.We put $\hbar = 1$, so that there is no distinction between $p = \hbar k$ and k. The dispersion law $\epsilon(k) \equiv \epsilon_k$ need not be quadratic, a general band shape is admitted, so that the kinetic energy of the electrons is $T = \sum |k\rangle\epsilon_k\langle k|$.

3. Physical concepts

While a true historical overview would be beyond the scope of this paper, it will be important to recall several fundamental ideas which run through the development of the transport theory. As will be seen, the physical principles of the contemporary NGF/Ansatz approach are not different from those which were on the minds of the founders of non-equilibrium statistical physics. The issues remain, the understanding and attitudes here changed. We choose just three topics.

I. The central idea of the transport theory has always been a ***reduced description*** of the system. The relevant information about a gas of particles was contained in the one-particle distribution function $f(x,p,t)$. The essential step was to search for a closed equation governing this function, that is for the transport equation. This was only possible, if, say, the description of binary collisions

in the gas was given in terms of the function f. As a systematic program, this seems to appear first in the work of Chapman and Enskog [26,27], but the principle dates back to Boltzmann himself [28–32], with his Stosszahlansatz for the binary distribution f_{12} expressed as $f_{12} \sim f_1 \times f_2$. This type of factorization, or, more generally, decoupling of higher correlation functions was systematically developed in the BBGKY technique. We have to say more about Bogolyubov, to whom we owe the postulate that *in a chaotized many-body system all higher particle correlation functions become a functional of the distribution function* [33–35,9,16,12]. Thus

$$f_{12} \overset{chaot.}{\longrightarrow} \Phi[f_1, f_2] \,. \tag{8}$$

The functional has yet to be specified, but this is of secondary importance. As will be described later, the KB Ansatz also singles out the one-particle distribution as the determining characteristic of the non-equilibrium system. This brings us to the ***reconstruction problem***: under which conditions the full description of the many-body interacting system can be built up from the knowledge of single-particle characteristics? This seemingly outrageous question was seriously treated in several contexts. In Section 8 we will discuss two of them: the time-dependent density functional theory (TDDFT), and the generalized Kadanoff–Baym Ansatz related techniques.

II. The second crucial notion is the ***hierarchy of characteristics times***. There are three intrinsic times related to a many-particle interacting system. In a reminiscence of a non-dilute gas, they are often identified as the *collision duration time* $\tau_c = a/\bar{v}$, the *collision time* $\tau_r = \ell/\bar{v}$ and the *hydrodynamic time* $\tau_h = L/\bar{v}$. Here, $\bar{v}$ is the average thermal velocity for a classical gas, the Fermi velocity v_F for a degenerate Fermi gas. The characteristic lengths are: a the interaction potential range (particle size), ℓ the mean free path (mean interparticle distance), and L the characteristic length of spatial inhomogeneities in the system. In the modern interpretation, the three times are: $\tau_c \cdots$ the chaotization time characterizing the decay of correlations, $\tau_r \cdots$ the relaxation time characterizing the thermalization of the system (local relaxation) and, finally, $\tau_h \cdots$ characterizes the process of relaxation of spatial inhomogeneities. In "normal" situations, the three times obey the inequality

$$\tau_c \ll \tau_r \ll \tau_h \tag{9}$$

separating the chaotization stage, the kinetic stage, and the hydrodynamic stage. This structuring of the spontaneous return to equilibrium was also introduced by Bogolyubov; he postulated Eq. (8) only for times later than the chaotization time τ_c. The Boltzmann equation proper corresponds to the limit

$$0 \leftarrow \tau_c \lll \tau_r \lll \tau_h \to \infty \,. \tag{10}$$

We will be mostly concerned with the opposite, more realistic case, when the distinction between τ_c and τ_r will be less sharp. Further, the time range of interest will be specified by the external fields. For example, an optical pulse is characterized by its duration, the ground period of the signal and its Rabi period measuring the pulse strength. These times should be compared with the intrinsic times of the system. This will, finally, specify the situation and the necessary version of transport theory used.

III. The last basic concept is that of the ***quasi-particles***. With this, we, as a matter of fact, move over to the quantum realm. There are several streams merging into the generalized notion of a quasi-particle. Firstly, the polaron, an electron dragging along a cloud of lattice polarization. In the quantum field language, the electron is dressed by virtual phonons. This compound object has some features characteristic of a particle, like a dispersion law (renormalized by the self-energy), which has an operational meaning in experiments. The self-energy is typically complex, and this leads to the finite life-time τ of the quasi-particles, closely related to the transport relaxation time τ_r. Secondly, and even more to the point, in a non-dilute system of interacting particles, their individuality is suppressed by mutual correlations and the use of a transport equation seems to be useless. However, the weakly excited states may appear to mimic a gas of weakly interacting quasi-particles. This was at the bottom of the Landau theory of the Fermi liquid [36], whose part was a proper adaptation of the Boltzmann equation [25,37]. This approximate, but highly precise description of

the Fermion systems had, of course, a number of predecessors, like the Sommerfeld electrons in simple metals, and parallels, like the quasi-particles in nuclei, where the self-energy has been originally introduced under the name of the optical potential. It might seem that the quantum transport equations for strongly interacting systems will all deal with the quasi-particles. This is, to some extent, true. However, the quasi-particles are vulnerable and elusive objects and cease to exist under some harsher conditions, like beyond the quasi-classical regime, for strong and/or transient disturbances, or if the system itself is not favoring their existence. This can sometimes be judged by the Landau–Peierls criterion [38]. Take the gas of quasi-particles with energies around the Fermi level E_F and a lifetime τ due to impurity scattering. The criterion reads: if $\tau \simeq \hbar/E_F$, the BE-like transport theory is not applicable. Now $\hbar/E_F$ can be interpreted as the "quasi-particle formation time" τ_Q. If$\tau \simeq \tau_Q$, the quasi-particle decays before having formed. On the other hand, τ is closely related to τ_r, whereas τ_Q appears to play the role of τ_c. The Landau–Peierls criterion thus states that if the quasi-particles do not form, then τ_r becomes comparable to τ_c and the condition Eq. (10) is not obeyed.

4. Origins: Boltzmann equation for classical and quantum particles

A prototype of all kinetic equations, the Boltzmann equation of classical physics [28–30,26,27,31,32,16,12] reads

$$\frac{\partial f}{\partial t} - \mathsf{drift}\,[f(t)] = I_{\rm in}[f(t)] - I_{\rm out}[f(t)]\,, \tag{11}$$

where the drift term is the classical Poisson bracket

$$\mathsf{drift}\,[f(t)] = \frac{\partial \varepsilon}{\partial k}\frac{\partial f}{\partial r} - \frac{\partial \varepsilon}{\partial r}\frac{\partial f}{\partial k}\,. \tag{12}$$

This is, in principle, an equation for a single-particle distribution function $f(k,r,t)$ in phase space, representing balance between the drift of particles (with energy $\varepsilon = \epsilon_k + U(r,t)$ and velocity $\frac{\partial}{\partial k}\,\varepsilon = \frac{\partial}{\partial k}\,\epsilon_k$ in the external force field $-\frac{\partial}{\partial r}\,\varepsilon = -\frac{\partial}{\partial r}\,U$), as given by the left-hand side of the BE, and the irreversible evolution due to collisions described by the scattering integrals $I_{\rm in}$ and $I_{\rm out}$ on the right-hand side. In these integrals, the collisions are approximated as instant randomizing events, so that the BE is Markovian. This is in agreement with the first inequality in Eq. (10). The other inequality demands all inhomogeneities in the system, including external fields, to be smooth enough to allow sufficient time for local equilibration.

The BE has been used for many classical systems and it was extended very early also to the transport by quantized particles, in particular, by electrons in metals. The quantum effects were incorporated mainly in the scattering integrals where the collision rates were calculated by the Fermi Golden Rule and the exclusion principle was taken into account by means of the Pauli blocking factors.

The average values of additive observables were calculated from formulas taken over from classical kinetic theory of gases. Thus, the particle density and the particle current density were

$$n(r,t) = \int \frac{\mathrm{d}k}{(2\pi)^3} f(k,r,t), \tag{13}$$

$$j(r,t) = \int \frac{\mathrm{d}k}{(2\pi)^3}\frac{\partial \epsilon}{\partial k} f(k,r,t). \tag{14}$$

Now, we depart from the BE in the direction towards quantum dynamic equations far from equilibrium. There are several extensions of the BE that we will first explore separately:

(i) From particles to quasi-particles. The interaction energy will no longer be negligible, but will be renormalized in the quasi-particle transformation.
(ii) From near-equilibrium to "arbitrary" non-equilibrium. This will be reflected in the memory of the system and taken into account by the non-Markovian GME.

5. Quasi-particles and transport

In dense systems, the particle interactions cannot be reduced to rare collisions randomizing the motion of otherwise free particles. Quantum

statistics for such systems at near-equilibrium are often well described by the Landau theory of quasi-particles. In this theory, weakly excited states of the interacting particles are described as a gas of quasi-particles with energy

$$\varepsilon(k,r,t) = \epsilon_k + U_{\text{eff}}(r,t) + \sigma(\varepsilon,k,r,t), \tag{15}$$

where U_{eff} may include the mean-field part of the interaction and the self-energy σ describes the mass renormalization. The quasi-particles are coupled by a weak residual interaction.

5.1. Quantum kinetic equation for quasi-particles

These quasi-particle features have consequences for transport properties, which are described by the Landau kinetic equation. It has the exact structure of BE (11). However, the energy entering the drift term is now the quasi-particle energy ε. Scattering integrals I_{in} and I_{out} contain scattering rates calculated again by the Fermi Golden Rule, but with the residual interactions reflecting that they are reduced by the many-particle wave–function renormalization. Finally, the function $f(k,r,t)$ is the *quasi-particle distribution function*.

Because of its intuitive character, the "Boltzmann" equation for quasi-particles provided many insights into the behavior of non-equilibrium many-particle systems. In particular, it offered a retrospective explanation of the over-successful Sommerfeld model of metals with non-interacting electrons responding to external fields. While various modifications of the BE-like approach have been applied successfully to many systems and situations, there are also many physical cases, in which it is bound to fail. The limitations of the Boltzmann equation include: (1) The BE well describes quantum systems if the quasi-particle picture is justified. This may no longer be valid in highly non-equilibrium quantum systems. (2) It is based on the intuitive idea of instant collisions between quasi-particles, which requires the collision duration time to be very short. (3) At the same time, the BE will not be well suited to describe systems with abrupt changes in space, including small structures, where quantum effects are essential and the quasi-classical approach hidden behind the BE is far from being sufficient [8,9,39,40].

5.2. Observables and quantum distribution function

Relations between the quasi-particle distribution function and the expectation values of observables are more complicated than (13) and (14). For example, the expression for current density must incorporate the back-flow accompanying the motion of quasi-particles. Rules for evaluating observables have been outset from an integral part of the Landau equilibrium theory. A natural question emerges: which is the relation between the quasi-particle distribution function f and the expectation values out of equilibrium?

Our task is then to find a functional relation

$$\{f,\ A\} \mapsto A_{\mathsf{A}v} = \text{tr}(\rho A),$$

which is equivalent to finding a functional $\rho[f]$ associating the single-particle density matrix with any given quasi-particle distribution. To relate the reduced density matrix ρ with the distribution function $f(k,r,t)$ it is convenient to express ρ in the (k,r) representation. This can be done in different ways, but we choose the so-called Wigner representation

$$\widetilde{\rho}(k,r,t) = \int \mathrm{d}x \mathrm{e}^{-\mathrm{i}kx} \rho\left(r + \frac{x}{2}, r - \frac{x}{2}, t\right). \tag{16}$$

The reduced density $\widetilde{\rho}(k,r,t)$ in the Wigner representation is commonly known by the name of Wigner distribution. It can be viewed as a distribution of electrons in the phase space and the expectation values

$$n(r,t) = \int \frac{\mathrm{d}k}{(2\pi)^3} \widetilde{\rho}(k,r,t), \tag{17}$$

$$j(r,t) = \int \frac{\mathrm{d}k}{(2\pi)^3} \frac{\partial \varepsilon}{\partial k} \widetilde{\rho}(k,r,t). \tag{18}$$

have the same form as in the Boltzmann theory.

These suggestive properties of the Wigner distribution should not lead us to the conclusion that this function is the "right" quantum generalization of the classical distribution function, and that the proper quantum generalization of the Boltzmann equation will be a kinetic equation of the Boltzmann form (11) for the Wigner

distribution function. We can see that this is not the case from the following argument given already by Landau.

Consider a homogeneous system. In equilibrium, the BE-like kinetic equation for electrons is solved by the Fermi–Dirac function regardless of the interactions in the system. Thus, at zero temperature, the distribution f jumps from 1 to 0 at the Fermi level. In contrast, the Wigner distribution describes the occupation numbers of true particles and it differs from the Fermi-Dirac function by depletion of the momentum states below the Fermi level. These missing states emerge as states above the Fermi level, where they form the so-called high-momenta tails of the Wigner function. The step of the distribution $\widetilde{\rho}$ is accordingly reduced to $1-2z$, where z is the renormalization constant for quasi-particles at the Fermi level.

We may summarize that the quasi-particle kinetic theory consists of two steps. First, the quantum kinetic equation is solved for the quasi-particle distribution. Second, the true quantum particle distribution is constructed by means of the functional $\rho[f]$ and the expectation values of the observables are calculated.

6. Generalized Master Equations: beyond the quantum kinetic equations

As already mentioned, quantum kinetic equations of the Boltzmann type have a restricted range of validity and these limits can be transgressed only by resorting to a more general framework, permitting, at least in principle, to start from a fully quantum description and work directly with an equation for the reduced density matrix (or the equivalent Wigner function), the so called quantum GME. There are several approaches and approximations leading to the GME [41–44,12,8,9], which has a general form

$$\begin{aligned} \frac{\partial\rho}{\partial t} - \mathrm{drift}[\rho(t)] &= \text{interaction term}, \\ \frac{\partial\rho}{\partial t} + \mathrm{i}[\underbrace{T+U_{\mathrm{eff}}(t)}_{H_0},\rho(t)]_- &= \int_{-\infty}^{t} d\bar{t} F[\rho(\bar{t})]\,. \end{aligned} \tag{19}$$

This equation is shown in an entirely symbolic form on the first line, and it is not actually explicit on the second one either. We will discuss the detailed structure of this type of equation below. Here, we only focus on its most salient features. The GME is a closed equation for ρ. It is non-Markovian, because the interaction term is non-local in time.

At the end of Section 5.1, we pointed out three important limiting factors for the use of the quantum kinetic equations. These factors will now be discussed from the point of view of the GME.

6.1. GME is an equation for ρ

Eq. (19) is a dynamical equation for the distribution of particles instead of quasi-particles as was the case of the BE. Therefore, it does not hinge on the use of quasi-particles, and it is free from the physical limitations necessary for introducing the gas of quasi-particles. In particular, the system may evolve under conditions which do not permit the quasi-particle states to consolidate. This does not preclude using some of the quasi-particle features where applicable. Thus, the left-hand side of the equation describes bare particles drifting under the influence of the effective field. All other features involving interactions are included in the right-hand side. It may be possible to transfer parts of the r.h.s to the drift term and achieve evolution in re-normalized bands.

6.2. Interaction term

We prefer to call the right-hand side of (19) on interaction term rather than scattering integrals. In principle, the GME is exact, so that the interaction term must incorporate all of the sub-dynamics of ρ reflecting not only particle collisions, but also the short time dynamics, off-shell propagation and coherence between the collisions and with the external fields, multiparticle correlations, gradual saturation of the scattering rates after the onset of a non-equilibrium process, etc.

It is remarkable that all this rich physics can be absorbed in an interaction term depending only on the one-particle density matrix. This is made possible by the subtle memory effect reflected in

the time integration over the full depth of the past in (19). Clearly, this form of the interaction term agrees with the Bogolyubov postulate quoted above in Section 3, at least for times beyond τ_c after the onset of the process. We will return to the related Reconstruction Theorems in Section 8.

6.3. Quasi-classical expansion

In the GME (19), neither the drift term, nor the interaction integral, are restricted to smooth variation of the fields and distributions in space. The drift term is given by the quantum Poisson bracket rather than by the classical one appearing in (12). For smooth functions, it can be quasiclassically expanded; the formal expansion parameter is $\hbar^2$. For the Wigner distribution $\widetilde{\rho}$ defined in Eq. (16), we obtain (writing, in the way of exception, the Planck constant explicitly):

$$\begin{aligned}\mathrm{drift}[\rho(t)] &= (i\hbar)^{-1}[T + U_{\mathrm{eff}}(t), \rho(t)]_- \longrightarrow \\ \mathrm{drift}[\widetilde{\rho}(t)] &= \frac{\partial\epsilon}{\partial p}\frac{\partial\widetilde{\rho}}{\partial r} - \frac{\partial U_{\mathrm{eff}}}{\partial r}\frac{\partial\widetilde{\rho}}{\partial p} \\ &\quad - \frac{\hbar^2}{3}\left(\frac{\partial^3\epsilon}{\partial p^3}\frac{\partial^3\widetilde{\rho}}{\partial r^3} - \frac{\partial^3 U_{\mathrm{eff}}}{\partial r^3}\frac{\partial^3\widetilde{\rho}}{\partial p^3}\right) + \ldots\end{aligned} \tag{20}$$

This expansion, suited for comparison of the GME in the quasiclassical limit with the corresponding kinetic equation is, in fact, a Fourier transformed expansion around the space diagonal $x_1 = x_2$.

7. NGF approach to non-equilibrium systems

This section only serves to introduce the concepts and relations concerning the NGF as they will be needed for our purposes, namely to derive and analyze the non-equilibrium dynamic equations of either the BE or the GME type. The formalism is commonly known today and there are a number of texts suitable for Refs. [3–9].

7.1. Green's functions on a time contour

In a short span of time, Schwinger and Martin [45,46,21], Kadanoff and Baym [3,22] and Keldysh [24,23] created the field theoretical perturbation scheme for the non-equilibrium Green's functions starting from causal Green's functions

$$\mathrm{G}(1,2) = -\mathrm{i}\langle\!\langle\, \mathbb{T}_{\mathrm{c}}[\psi(1)\psi^{\dagger}(2)] \,\rangle\!\rangle \tag{21}$$

with the time-ordering operator $\mathbb{T}_{\mathrm{c}}$ acting on a time contour $\mathbb{C}$. Here, in Fig. 1 we illustrate the Schwinger contour, usually referred to as the Keldysh contour.

The rightmost turning point, just like the terminal point t_0 is usually sent to $+$ or $-$ infinity; we prefer to keep t_0 finite to make contact with the problem of the initial conditions otherwise eliminated by the limit $t_0 \to -\infty$. For given times t_1, t_2, there are four different orderings on the $\mathbb{C}$ contour, as shown in the figure, and an equivalent formalism working with a matrix Green function of real times running from $-\infty$ to $+\infty$,

$$\overset{\supset}{\mathbf{G}} \equiv \begin{bmatrix} G^c & G^< \\ G^> & \widetilde{G^c} \end{bmatrix} \tag{22}$$

can be established. Here, $G^c = -\mathrm{i}\langle\!\langle\, \boldsymbol{T}[\psi\psi^{\dagger}] \,\rangle\!\rangle$ and $\tilde{G}^c = -\mathrm{i}\langle\!\langle\, \tilde{\boldsymbol{T}}[\psi\psi^{\dagger}] \,\rangle\!\rangle$ are the usual causal and anti-causal GF's of real times, while

$$\begin{aligned} G^>(1,2) &= -\mathrm{i}\,\langle\!\langle\, \psi(1)\psi^{\dagger}(2) \,\rangle\!\rangle \\ G^<(1,2) &= +\mathrm{i}\,\langle\!\langle\, \psi^{\dagger}(2)\psi(1) \,\rangle\!\rangle \end{aligned} \tag{23}$$

differ only by factors of i from $g^<$, $g^>$ as defined in Eqs. (5) and (7). Sometime, it may be convenient to embed the $\mathbb{C}$ contour in the complex time plane in order to use the procedure of analytical continuation to link the contour with the Matsubara imaginary line [3]. In general, however, the contour has an entirely symbolic meaning.

Only two of the four functions (22) are independent. Kadanoff and Baym took for these two functions $G^>, G^<$ and developed their KB formalism [3]. In parallel, Keldysh created a basically equivalent matrix formulation of the

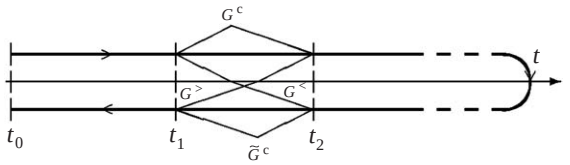


Fig. 1. NGF time contour.

NGF approach. There is quite a choice among the variants of these two approaches [3–9]. To retain the matrix structure of the equations, a slightly redundant set of three functions is needed. We will use a modified Keldysh formulation suggested by Langreth and Wilkins [47,48]. It is obtained by a linear transformation

$$\overset{\supset}{\mathbf{G}} \mapsto \mathbf{M}\boldsymbol{\sigma}_z \overset{\supset}{\mathbf{G}}\, \mathbf{M}^{-1} \equiv \mathbf{G} \tag{24}$$

with

$$\mathbf{M} = \begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix},\ \boldsymbol{\sigma}_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}. \tag{25}$$

Result:

$$\mathbf{G} = \begin{bmatrix} G^{\mathrm{R}} & G^{<} \\ 0 & G^{\mathrm{A}} \end{bmatrix}. \tag{26}$$

The transformed set consists of Green's functions including $G^{<}$ and the retarded and advanced propagators G^{R}, G^{A} defined by the identities

$$\begin{aligned} &G^{c}(1,2) - G^{<}(1,2) = G^{\mathrm{R}}(1,2), \\ &G^{c}(1,2) - G^{>}(1,2) = G^{\mathrm{A}}(1,2), \\ &\tilde{G}^{c}(1,2) - G^{<}(1,2) = -G^{\mathrm{A}}(1,2), \\ &\tilde{G}^{c}(1,2) - G^{>}(1,2) = -G^{\mathrm{R}}(1,2). \end{aligned} \tag{27}$$

Explicitly,

$$G^{\mathrm{R}}(1,2) = \theta(t_1 - t_2)(G^{>}(1,2) - G^{<}(1,2)), \tag{28}$$

$$G^{\mathrm{A}}(1,2) = -\theta(t_2 - t_1)(G^{>}(1,2) - G^{<}(1,2)). \tag{29}$$

Keldysh used the set G^{R}, $G^{<} + G^{>}$, G^{A} instead [24].

The fourth GF is expressed in terms of the triplet through the obvious but important "spectral identity"

$$\begin{aligned} G^{\mathrm{R}}(1,2) - G^{\mathrm{A}}(1,2) &= G^{>}(1,2) - G^{<}(1,2) \\ &\equiv -\mathrm{i}A(1,2). \end{aligned} \tag{30}$$

The triplet is overcomplete, as there holds the conjugation $G^{\mathrm{R}}(1,2) = [G^{\mathrm{A}}(2,1)]^{*}$ (any of the three functions G^{R}, G^{A}, *the spectral density*, is fully equivalent to the other two). A further reduction to a single GF is only possible in equilibrium.

The set G^{R}, $G^{<}$, G^{A} arranged to the upper triangular matrix $\mathbf{G}$ is extremely useful in algebraic manipulations. As a basic and typical example consider the product $[\Sigma \mathrm{G}]_{\mathrm{C}}$ on the contour. In the matrix form, it is given by

$$\begin{aligned} \boldsymbol{\Sigma}\mathbf{G} &= \begin{bmatrix} \Sigma^{\mathrm{R}} & \Sigma^{<} \\ 0 & \Sigma^{\mathrm{A}} \end{bmatrix} \cdot \begin{bmatrix} G^{\mathrm{R}} & G^{<} \\ 0 & G^{\mathrm{A}}. \end{bmatrix} \\ &= \begin{bmatrix} \Sigma^{\mathrm{R}} G^{\mathrm{R}} & \Sigma^{\mathrm{R}} G^{<} + \Sigma^{<} G^{\mathrm{A}} \\ 0 & \Sigma^{\mathrm{A}} G^{\mathrm{A}} \end{bmatrix}. \end{aligned} \tag{31}$$

These are the "Langreth-Wilkins" rules in a compact form [47,48]: the retarded (1,1) component contains only R–factors, similar to the advanced component (2,2). The $<$ ("*less*") (1,2) component is a sum of all possible products with factors in the causal order $\mathrm{R}\cdots<\cdots\mathrm{A}$. These rules hold for any number of factors (chain rule). It is important that the *less* component of the product is necessarily linear in the *less* quantities. In an explicit form, all products are integral over the internal variables, like

$$\begin{aligned} [G^{\mathrm{R}}\Sigma^{<}](1,2) &= \int \mathrm{d}3 G^{\mathrm{R}}(1,3)\Sigma^{<}(3,2) \\ &\equiv G^{\mathrm{R}}(1,\bar{3})\Sigma^{<}(\bar{3},2). \end{aligned}$$

7.2. Explicit construction of the NGF

Up to now, the procedure of introducing the NGF has been formal, but wholly general. It offers no practical means of constructing an actual GF for a specific situation. We have to recall that the $\langle\!\langle \cdots \rangle\!\rangle$ average means, in fact, $\mathrm{TR}(\hat{\rho}\cdots)$, where the many-body initial state $\hat{\rho}$ at $t = t_0$ has so far been arbitrary. If, say, a perturbation expansion in the powers of the interaction is intended, the initial state should belong to an unperturbed Hamiltonian quadratic in the quantum fields; this is barely the case for any finite t_0, and we have to resort to the usual limit $t_0 \to -\infty$ associated with the assumption of the "decay of initial correlations", another of the Bogolyubov tenets. This is the Keldysh way [24,5,25]. Alternatively, the trajectory may be bent along the Matsubara interval $\langle t_0, t_0 - \mathrm{i}\beta\rangle$ in the complex plane, but again with $t_0 \to -\infty$. This is the Kadanoff–Baym variant [3]. All other, more general situations amount to dealing with the so-called problem of *correlated initial conditions*,

which has been treated by a number of authors [49–63]. Less attention has been paid so far to the connection between the initial conditions and the construction of the transport equations [55,56,60]. This is natural for a steady transport: the initial correlations die out while the steady regime sets on. The situation may dramatically differ for fast transients and most of Paper III will deal with the related questions.

Here, we prefer to concentrate on the basic Ansatz formulation and on the related reconstruction problem. Therefore, we will only deal with the physical situations, in which the initial conditions pose no additional problems. Specifically, we restrict our considerations to the class of the so-called *switch-on states*, that is, we start from an equilibrated state disturbed subsequently by an external field.

In this equilibrium starting state including the interactions, there exists an unperturbed state, as required by the principle of weakening of initial correlations. The two states could be linked by an equilibrium perturbation scheme. It is preferable to first act on this unperturbed state by the (effective) external field. This permits to introduce the *reference unperturbed field-dependent NGF matrix* $\mathbf{G}_0$ incorporating already the required boundary conditions. Finally, we turn to the interactions by a non-equilibrium technique. The resulting full NGF defines the self-energy matrix from the Dyson equation

$$\mathbf{G} = \mathbf{G}_0 + \mathbf{G}_0 \boldsymbol{\Sigma} \mathbf{G}, \tag{32}$$

which can be handled by the LW rules, etc.

To close the equations, it is necessary to specify the (approximate) self-energies $\Sigma^<$, $\Sigma^{\mathrm{R,A}}$. For a consistent transport theory, it is important to express these in terms of Green's functions themselves, that is, to use a self-consistent approximation. To be physically correct, the approximation should further obey the basic requirements, like the symmetry laws, conservation laws, causal structure, etc.

We will not discuss specific approximations for the self-energies, assuming that the self-energies in question are physically consistent, so that the related Green's functions can serve as a basis for constructing transport equations for quantum distribution functions.

7.3. Dyson equations for propagators; self-energies

By the LW rules, the non-equilibrium propagators $G^{\mathrm{R,A}}$ satisfy the usual Dyson equations. Written in the symmetric differential form

$$\{G^{\mathrm{R,A}}\}^{-1} = G_0^{-1} - \Sigma^{\mathrm{R,A}}, \tag{33}$$

they serve, in fact, as defining identities for the respective self-energies. We have to specify the free Green's functions $G_0^{\mathrm{R,A}}$. As indicated in (33), they have a common inverse G_0^{-1}. In agreement with (32), it is defined as incorporating the *effective* external field augmented by the mean-field contributions to the potential energy,

$$G_0^{-1}(1,2) = \delta(1-2)\left(\mathrm{i}\frac{\partial}{\partial t_2} - \epsilon\left(\frac{1}{\mathrm{i}}\nabla_2\right) - U_{\mathrm{eff}}(x_2,t_2)\right). \tag{34}$$

The self-energy Σ is cleared of the mean field, that is of a "singular" time-local component, by this definition. There are altogether four combinations as differential or integral Dyson equations corresponding to (33); we quote one of them for reference:

$$G_0^{-1} G^{\mathrm{R}} = I + \Sigma^{\mathrm{R}} G^{\mathrm{R}}, \tag{35}$$

$$G^{\mathrm{R}} = G_0^{\mathrm{R}} + G_0^{\mathrm{R}} \Sigma^{\mathrm{R}} G^{\mathrm{R}}\ . \tag{36}$$

Here, $I(1,2) = \delta(1-2)$. The effective external fields and the boundary conditions, that is, the jump conditions at equal times (from zero to $-\mathrm{i}$ for G^{R}, from $+\mathrm{i}$ to zero for G^{A}) enter the problem through the free propagators $G_0^{\mathrm{R,A}}$. The integral Dyson equation serves the important purpose of transmiting these properties on the full propagators.

7.4. Dyson equation for $G^<$

Equation of motion for the correlation function $G^<$ will play a central role in this paper. It is convenient to start from its differential form. To this end, we left-multiply Eq. (32) by $\mathbf{G}_0^{-1}$ and then take the *less* component. Employing (33), we finally obtain the first of the following two

conjugate integro-differential equations of motion for $G^<$, valid for times $t_1 > t_0$, $t_2 > t_0$:

$$\{G^R\}^{-1} G^< = \Sigma^< G^A, \tag{37}$$

$$G^< \{G^A\}^{-1} = G^R \Sigma^<. \tag{38}$$

These equations are fully renormalized. We have to treat the initial/boundary condition with great care. Either we perform the limit $t_0 \to -\infty$, or we decide to keep t_0 finite. Then, at variance with the propagators, the initial condition does not just reduce to a unit jump at equal times. Instead, the conditions at an initial time t_0 have to be specified (do not mix this unfortunate "0" with that of the free propagators). In the simplest case, taken into consideration by Keldysh and corresponding neatly with the transport equation approach, the initial condition is assumed as *uncorrelated* and reduces to the knowledge of the one-electron density matrix

$$\rho(t_0) = \rho_{\text{init}}. \tag{39}$$

In that case, $G^<$ has the form, frequently called the Dyson–Keldysh Equation,

$$G^< = G^R \wp^<_{\text{init}} G^A + G^R \Sigma^< G^A, \tag{40}$$

where

$$\wp^<_{init}(1,2) = \mathrm{i}\delta(t_1 - t_0)\delta(t_2 - t_0)\rho_{\text{init}}(x_1, x_2). \tag{41}$$

In the general case of correlated initial conditions, two additional terms containing contributions to the self-energy singular at t_0 would contribute to the full $G^<$ see Paper III and Refs. [4,62].

Eq. (40) with all integrations explicitly shown reads

$$G^<(1,2) = \int_{t_0}^{t_1} d3 \int_{t_0}^{t_2} d4\, G^R(1,3)\, \wp^<_{\text{init}}(3,4) G^A(4,2) + \int_{t_0}^{t_1} d3 \int_{t_0}^{t_2} d4\, G^R(1,3) \Sigma^<(3,4) G^A(4,2). \tag{42}$$

The first line involves, in fact, no time integrations; by (41), its structure is

$$\mathrm{i} G^R(t_1, t_0) \rho_{\text{init}} G^A(t_0, t_2).$$

This term describes coherent evolution and gradual decay of the initial condition; for free particles, this would be the complete $G_0^<$. The other term, associated with the steady stage of the transport processes gradually takes over. In fact, in the long time limit $t_0 \to -\infty$ (...kinetic regime), the first term of (40) will die out and only the second term of the Dyson–Keldysh Equation will survive.

While this integral form attributed to Keldysh is very illuminative concerning the causal structure of the theory and will be handy in formal manipulations, it is prohibitively complex for numerical work. A practicable form of a closed transport theory at the level of double-time non-equilibrium correlation functions is based on a (numerical) solution of the pair of coupled integro-differential equations, say (36) and (37) with the initial condition (39). The other propagator G^A is found by conjugating G^R. This is an alternative to the basic KB theory working in the same way with equations for $G^>, G^<$.

7.5. Precursor equation

To continue from the NGF to transport equations for the quantum distribution function, we use, instead of (37) or (38), their difference,

$$\{G^R\}^{-1} G^< - G^< \{G^A\}^{-1} = -G^R \Sigma^< + \Sigma^< G^A, \tag{43}$$

while retaining the Dyson equation for the propagators. The new equation is commonly called the *precursor transport equation*, because it already has a structure closely related to transport equations. Using Eq. (33), it can be rewritten with an unrenormalized drift on the l.h.s.:

$$G_0^{-1} G^< - G^< G_0^{-1} = -G^R \Sigma^< + \Sigma^< G^A + \Sigma^R G^< - G^< \Sigma^A, \tag{44}$$

Employing (6), (34), we find the l.h.s. of the last equation at equal times:

$$\text{l.h.s. of (44)} \xrightarrow{t_1 = t_2} \frac{\partial \rho}{\partial t} + \mathrm{i}[H_0, \rho]_- . \tag{45}$$

This part of the equation has, thus, the form of the GME. The "interaction terms" on the r.h.s., however, are expressed by means of the double-time

quantities. Our aim will be a reduction of these terms to expressions specified by a single time distribution function, ρ in the case of the GME.

To obtain a kinetic equation involving the quasi-particle distribution f, we will have to proceed in a modified way. In particular, the drift term on the l.h.s. will be partly renormalized, that is, it will be somewhere between the fully renormalized drift in (43) and the bare drift in (56).

Note on Dyson equations for $g^<$

There are reasons to favor one or the other convention as regards the correlation functions. Unfortunately, here we have to quote both: for historical reasons, use of $g^<$, $g^>$ became common in papers concerning the quantum kinetic equations and the KBA. On the other hand, the GME, as a systematic tool preserving the innate structure of the NGF formalism, is more closely connected to the $G^<$, G^A choice. In agreement with this, we will use different conventions in Papers II and III.

With the relations (compare Eqs. (5), (7) with Eq. (23) as discussed already in Section 7.1),

$$G^<(1,2) = \mathrm{i}g^<(1,2), \tag{46}$$

$$G^>(1,2) = -\mathrm{i}g^>(1,2), \tag{47}$$

we have, for example,

$$G^R(1,2) = -\mathrm{i}\theta(t_1 - t_2)(g^>(1,2) + g^<(1,2)), \tag{48}$$

$$G^A(1,2) = \mathrm{i}\theta(t_2 - t_1)(g^>(1,2) + g^<(1,2)). \tag{49}$$

We recall that in the Langreth–Wilkins formalism, all equations are necessarily linear in the "less" quantities, while there is no such limitation on the propagator-related quantities. As a result, all previous results for $G^<$, $\Sigma^<$ are easily transformed to a form appropriate for $g^<$. The correlation functions were related by (46), (47). Extending the same definition also to the self-energies and to the initial condition, that is, writing

$$\Sigma^<(1,2) = \mathrm{i}\sigma^<(1,2), \tag{50}$$

$$\Sigma^>(1,2) = -\mathrm{i}\sigma^>(1,2), \tag{51}$$

$$\wp^<(1,2) = \mathrm{i}\rho^<(1,2), \tag{52}$$

we obtain equations equivalent to (40) and (37), (38):

$$g^< = G^R\rho^<_{\mathrm{init}}G^A + G^R\sigma^<G^A, \tag{53}$$

and

$$\{G^R\}^{-1}g^< = \sigma^<G^A, \tag{54}$$

$$g^<\{G^A\}^{-1} = G^R\sigma^<. \tag{55}$$

Finally, for the precursor equation we obtain

$$-\mathrm{i}\big(G_0^{-1}g^< - g^<G_0^{-1}\big) = \mathrm{i}\big(G^R\sigma^< - \sigma^<G^A\big) - \mathrm{i}\big(\Sigma^Rg^< - g^<\Sigma^A\big). \tag{56}$$

8. The reconstruction procedure

The general plan of generating quantum transport equation within the NGF scheme is to take the precursor transport equation in one of its forms (43), (44) and (56), and to express the precursors to scattering (interaction) integrals in terms of one or the other distribution function. This will transform the equation involving two-point GF to a transport equation having the single-point distribution function as the unknown. For the purpose of this transformation, one of the approximate "Ansatzes" will be used, as outlined in Section 1. We wish to outline this approach in the present paragraph concentrating on the associated general questions. One basic question is: what is the real justification for such a round-about way to the transport equations? In other words, what is gained by working this way, compared to other approaches?

Viewed from another angle, we may detach the construction of the transport equations from the fundamental issue that we already summarized as the hypothetical Reconstruction Theorem. To recapitulate the situation, it appears natural that virtually all of the relevant information about a non-equilibrium many-body system can be unfolded from its reduced characteristics, namely a pair of two-point quantities, say $G^<$ and $G^>$. The Bogolyubov principle (8), just as the Ansatzes hint at the possibility that, actually, it may be enough to know or control even less, just a function of a single time variable, the one-particle density

matrix, or even a one-point quantity, the local particle density. Thus, the ***reconstruction problem*** of Section 3 can be made more specific: under which conditions the full description of the many-body interacting system can be built up from the knowledge of its *single-time single-particle characteristics*?

It should be cautioned already here, however, that any Ansatz scheme in practical use, be it Kadanoff–Baym Ansatz, Generalized Kadanoff–Baym Ansatz, or any of their variants, plays the role of a physically well-justified, but still approximate truncation of the NGF. This would make the reconstruction procedures approximate already by their nature. Another problem occurring in the Ansatz schemes is that the knowledge of the distribution function alone is not sufficient: the additional quantities entering the equations are propagators, and it has to be clarified, whether they are generated from the known distribution function in a separate step, or whether they are entering the scheme as an independent input, difficult to obtain beyond an approximation. Last but not least, we again have to caution that it is rather difficult to extend an Ansatz procedure so as to incorporate correlated finite-time initial conditions. These problems of principle have, of course, only a limited significance for practical use of the Ansatz technique, if it turns out to be convenient and gives reliable results.

Let us have a look at the status of some alternative approaches *vis-à-vis* the reconstruction problem. Only then, will we be able to formulate the reconstruction hypothesis properly.

First, the BBGKY method of an infinite chain of equations for reduced density matrices of all orders is inherently associated with a decoupling (truncation) in the chain [12,42–44,9]. This certainly leads to a reduced description, but the whole approach is not directly related to the reconstruction problem in the narrow sense followed here.

Second, the projection methods in the Liouville space are a more likely candidate [64–70]. A partitioned expression for the projected (relevant) density matrix is closed and exact, in principle. It is open to generating ever-improving approximations in a systematic way. The difficulty with this approach is its complexity, which exceeds that of the NGF method. There are some very important developments aiming at a combined technique permitting to take advantage from both sides, and, in particular, to extend the GF methods directly to systems with open boundary conditions at finite times [71–73].

There is a third, truly likely contender, the Time Dependent Density Functional Theory (TDDFT) [74–76]. In fact, some of the general results obtained in the context of this approach are about closest to the fundamental formulation of the Reconstruction Problem. At the same time, TDDFT draws from an independent source of physical inspiration. In view of this, we devote a paragraph to the TDDFT before discussing our main subject, the Ansatz approach.

8.1. Functional substitution: inspiration by TDDFT

A well-known case of functional substitution, seminal for the present topic, is the Hohenberg–Kohn Theorem concerning equilibrium many-body systems [76–78]. Their equilibrium state is specified by the time independent external field $U(r)$ acting on the system. In particular, the local particle density $n(r)$ depends on $U(r)$. The two functions are *dual*: they enter the total energy $\langle\!\langle \hat{H} \rangle\!\rangle$ of the system as the bilinear functional $\langle U \rangle = \int \mathrm{d}^3 r\, n(r) U(r)$. This suggests a functional substitution $U \to n$ permitting to formulate the whole many-body problem as depending on the new functional variable. The theorem claims that such a substitution is possible— under conditions we do not care to elaborate. The new energy functional is obtained by the Legendre transformation as $E(n) = \langle\!\langle \hat{H} \rangle\!\rangle - \langle U \rangle$, which has been given on a firm mathematical basis [78,79].

As has been pointed out already in [17], " ... the feasibility of an exact building up of the full correlation functions from their time-diagonal sections can be motivated on physical grounds resembling somewhat the reasoning leading to the Hohenberg–Kohn theory." It became clear over the time that the non-equilibrium analogue of the Hohenberg–Kohn Theorem will be far more complicated: non-stationary dynamics of a many-body system is specified by two groups of physical constituents, the initial conditions and the driving

forces. Let us consider the simplest, and simultaneously the particularly important case of the switch-on states. The first group, the initial condition, then concerns the system in equilibrium and includes the particle types and numbers, the-many-body interactions and the boundary conditions given by the thermodynamic environment. The second group, barring non-mechanical perturbations, consists of only one, but crucial member; the external field $U(x,t)$ acting from the initial time t_0 on. This external field uniquely specifies each non-stationary mechanical process in the system. It enters the NGF formulation through the free Green's function G_0, Eq. (34). All quantities including the full Green's functions are functionals of the external field. The function dual to the space- and time local field $U(1)$ is now given by the bilinear functional $\int \mathrm{d}1\, n(1)U(1)$ as the particle density $n(1)=\rho(1,1)$. It is natural, but premature, to expect that the functional substitution $U \to n$ will also work in the non-equilibrium case, although this expectation has been a tacit assumption of the TDDFT for a long time.

A firm basis for the subsequent development of the TDDFT is given by the Runge–Gross Theorem [80,74–76]. It plays the exactly role of the Kohn–Hohenberg Theorem, namely it is an existence theorem. It states that, for any initial condition specified by a pure many-body state Ψ_0 at the initial time t_0, different external fields $U(1)$ induce different local particle densities $n(1)$, so that the substitution $U \to n$ is justified. (The fields U must be Taylor expandable in time at each time point). Here, we do not describe the specific problems of the TDDFT, connected to the time-dependent Kohn-Sham formalism of equivalent ghost systems of non-interacting particles. The Runge–Gross Theorem has a much wider applicability, however.

One nice point is that the Theorem provides a proof of the Bogolyubov conjecture quoted in Section 3, at least for a class of typical physical situations, which is not overly specialized. In fact, the Theorem implies even more, because the reduction to the one-particle distribution applies right from t_0, while the Bogolyubov postulate allows for a formation time τ_c which must elapse before the reduction takes place. This notion is physically appealing, and it would be interesting to study the early Runge–Gross evolution of the system in more detail.

It should be stressed that an entirely arbitrary initial condition *cannot* be uniquely characterized by its one-particle reduced characteristics. This is reflected in the formulation of the Theorem, of course. We may note that the situation is similar to the one we have already encountered in connection with the correlated initial condition for the NGF. There, we have singled out three special classes of simple initial conditions: the uncorrelated initial condition at $t_0 \to -\infty$ (the Bogolyubov decay of *initial* correlations), the finite t_0 initial condition uncorrelated by assumption (Keldysh IC) and the switch-on states. The last case is particularly appealing: the initial state is generated by a perturbation of a "dark" (*i.e., no field*) state in a distant past. If this dark state is a state of equilibrium, the Hohenberg–Kohn Theorem applies; then, the state evolves under the conditions of the Runge–Gross Theorem. Consequently, here we encounter an initial condition fully reducible to the history of $n(r,t)$ for t preceding t_0.

The last point of this section focuses on the actual implementation of the functional substitution. The original idea to base it on the real time Legendre transform $\int \mathrm{d}1\, n(1)U(1)$ encountered inconsistencies, as mentioned above. As could have been expected, an adequate description of the non-equilibrium dynamic states calls for the use of the Schwinger–Keldysh trajectory, so that the proper modification of the functional becomes

$$\int_{\mathbb{C}} \mathrm{d}1\, n(1)U(1) = \langle \Psi_0 | \int_{\mathbb{C}} \mathrm{d}1\, \hat{n}(1)U(1) | \Psi_0 \rangle \equiv \langle\!\langle \int_{\mathbb{C}} \mathrm{d}1 \hat{n} U \rangle\!\rangle .$$

Recognition of this integration path was one of the key steps in developing the contemporary TDDFT and linking it with the NGF language and technique [75,81]. For all details on this extensive and developing field, the reader is referred to reviews and to original papers. It is rewarding to observe that by this development, two major branches of the Schwinger school, the DFT as

represented by W. Kohn, and the NGF with the Schwinger–Martin–Kadanoff & Baym/Horing pedigree [21,82,81], converge together in one major contemporary direction of many-particle/condensed matter theory.

8.2. Intuitive way to reconstruction: Kadanoff–Baym Ansatz

To physically motivate the general formulation of the reconstruction problem in the context of the NGF based transport theory, we will introduce the historically first solution of the reconstruction problem and stress some of its important features. This was proposed by Kadanoff and Baym in 1962 [3], when they aimed at the construction of a quantum Boltzmann equation from the KB equations for $g^<$ and $g^>$. Their approach thus did not strive for generality. They rather made two appropriate assumptions: (i) The disturbance $U(1)$ had to vary slowly both in space and time. (ii) The excited states engaged in the transport process were to be stable quasi-particles.

Here, we will not follow the original work, but rather show, without detailed references, how this line of thinking developed over time. The two assumptions are formalized in two steps. First, the transition to the Wigner representation for all four space-time variables is made. For any two-point function, $F(1, 2)$, we make the transformations

$$\begin{aligned}[x_1,t_1],[x_2,t_2] &\to [r=\frac{1}{2}(x_1+x_2), t=\frac{1}{2}(t_1+t_2)],\\ &\quad [\bar{x}=x_1-x_2, \bar{t}=t_1-t_2]\\ F(x_1;t_1,x_2;t_2) &\to F(r+\frac{1}{2}\bar{x};t+\frac{1}{2}\bar{t},r-\frac{1}{2}\bar{x};t-\frac{1}{2}\bar{t})\\ &\xrightarrow{F.T.} f(k,\omega,r,t) \end{aligned} \tag{57}$$

This leads to the notion of a local electron structure, slowly dependent on the changing average position r and time t. In the second step, Eq. (55) for $g^<$ is written in the Wigner (mixed) representation and all damping terms are left out, accounting for the assumption of stable quasi-particles:

$$\big[\omega-\epsilon_k-U_{\mathrm{eff}}(r,t)-\sigma(k,\omega,r,t)\big]g^<(k,\omega,r,t)=0. \tag{58}$$

We use the shorthand $\sigma=\mathrm{Re}\,\sigma^{\mathrm{R}}$, see Eq. (II.14) in Paper II. The general solution of this equation is

$$\begin{aligned} g^<(k,\omega,r,t) &= \phi(k,\omega,r,t)\\ &\quad\times\delta\big(\omega-\epsilon_k-U_{\mathrm{eff}}(r,t)-\sigma(k,\omega,r,t)\big), \end{aligned} \tag{59}$$

where the second δ-factor allows in the present case to define the local quasi-particle dispersion law by

$$\varepsilon(k,r,t)=\epsilon_k+U_{\mathrm{eff}}(r,t)+\sigma(k,\omega,r,t)\big|_{\omega=\varepsilon(k,r,t)}, \tag{60}$$

while the first factor is an arbitrary function. Finally, solution (59) assumes the form, which will presently be termed the *Kadanoff–Baym Ansatz*:

$$\begin{aligned} g^<(k,\omega,r,t) &= f(k,r,t)\times\delta(\omega-\varepsilon(k,r,t)),\\ f(k,r,t) &= \left[\frac{1}{1-\frac{\partial\sigma}{\partial\omega}}\phi(k,\omega,r,t)\right]_{\omega=\varepsilon(k,r,t)}. \end{aligned} \tag{61}$$

Here, $\delta(\omega-\varepsilon(k,r,t))$ obviously plays the role of the quasi-particle spectral function $A_{\mathrm{Q}}(\omega,k,r,t)$. It is then natural, and later will be verified, that the function f should be identified with the quasi-particle distribution. In Paper II, this identification will be made by employing (61) in the precursor equation (56) and demonstrating that f obeys the quantum kinetic equation.

Here, we link (61) with the Fluctuation Dissipation Theorem rewritten for $g^<$ in the form

$$\begin{aligned} g^<(k,\omega,r,t) &\overset{equil.}{\equiv} g^<(k,\omega)\\ &= f_{\mathsf{FD}}(\omega)\times A(k,\omega). \end{aligned} \tag{62}$$

This identity is strictly an equilibrium feature and reduces the number of independent Green's functions to one: $f_{\mathsf{FD}}(\omega)$ is the Fermi–Dirac factor, a univeral function of energy. If A is replaced by A_{Q}, we obtain the equilibrium limit of (61) with

$$f(k,r,t)\equiv f(k)=f_{\mathsf{FD}}(\varepsilon(k)) \tag{63}$$

This is precisely the equilibrium quasi-particle distribution. We see that the Kadanoff–Baym Ansatz can be viewed as a non-equilibrium extension of the Fluctuation Dissipation Theorem to locally equilibrated states, suitable not very far from equilibrium. In qualitative terms, beyond equilibrium, the two functions $g^<$ and A are not

completely reduced one to another: additional information, the quasi-particle distribution f, is required. Still, $g^<$ plus A can be *reconstructed* from a substantially reduced information contained in f plus A.

To gain a better feeling of the cavalierly interchanges $A \longleftrightarrow A_{\rm Q}$, let us introduce the renormalization constant z and rewrite the exact equilibrium particle spectral density as

$$A(k,\omega) = z(k)\delta(\omega - \varepsilon(k)) + \text{SATELLITES}$$
$$z(k) = \frac{1}{1 - \frac{\partial\sigma}{\partial\omega}\Big|_{\omega=\varepsilon(k)}}. \tag{64}$$

Let us try to leave out the satellite contribution. This permits to rewrite (62) in two "improved" KBA- like ways:

$$g^< = f \times z \times \delta(\omega - \varepsilon) \overset{?!}{=} \begin{cases} \overbrace{f}^{\text{QP}} \times \overbrace{z \cdot \delta(\omega - \varepsilon)}^{\text{particle } A} \\ \underbrace{f \cdot z}_{\rho} \times \underbrace{\delta(\omega - \varepsilon)}_{\text{QP } A_{\rm Q}}. \end{cases} \tag{65}$$

Here, the particle correlation function $g^<$ factorizes either to the QP distribution times the true spectral function (upper line), or to a product of the particle distribution and the QP spectral function (lower line). In either form, a most important aspect of the true Kadanoff–Baym Ansatz is lost, namely an automatic particle number conservation. This is achieved, in the KBA, by lumping together the satellite fraction $1 - z$ of the spectral weight with the z weight of the quasi-particle resonance. Clearly, a better treatment of the satellites is desirable. This leads to the concept of the *extended quasi-particles* explained in Paper II.

Another important comparison between the Fluctuation Dissipation Theorem (63) and its KBA extension (61) is best made in the original space–time representation (only the time arguments are shown for clarity):

$$G^<(t_1,t_2) = f(\frac{t_1+t_2}{2})[G^{\rm A}(t_1,t_2) - G^{\rm R}(t_1,t_2)], \tag{66}$$

where the spectral function is written as $A = \mathrm{i}(G^{\rm A} - G^{\rm R})$, see (30). In correspondence with the quasi-classical nature of the KBA, the quasi-particle distribution is taken at the mid-point time $t = \frac{1}{2}(t_1 + t_2)$. This feature violates the overall causal structure of the NGF theory manifested in Eqs. (40) and (42). If the Ansatz is to consistently extend the distribution function to $G^<$, the distribution should appear as an initial condition of its kind at the earliest time and then be propagated to later times. In Section 4 of Paper II we will discuss how the acausal features of the KBA are closely related to the description of the particle collisions in the quantum BE. The KBA time structure (66) becomes very disturbing beyond the quasi-classical limit, and this was one of the reasons for introducing the so-called GKBA, which was constructed to be causal from the outset. This Ansatz is the subject matter of Paper III. The basic ideas leading to the GKBA and from there to the "Reconstruction Theorem" will be outlined, in the next subsection.

8.3. From GKBA to the Reconstruction Theorem

The GKBA has been introduced as an alternative to the original KBA [17–20,8,9]. It can be written as

$$G^<(t_1,t_2) = -G^{\rm R}(t_1,t_2)\rho(t_2) + \rho(t_1)G^{\rm A}(t_1,t_2), \tag{67}$$

In comparison with the KBA, as given by (66), it differs in terms of four constitutive properties:

Causal structure: The two propagators are now separated and each is multiplied by its own distribution function corresponding to the earlier time argument, depending on the retarded or advanced propagation

Equal time limit: The distribution function is the true one-particle density matrix, not the quasi-particle distribution. Thus, at equal times, the GKBA for $G^<$ obeys identity (6). This implies an automatic particle number conservation.

General representation: The order of factors corresponds to the products interpreted as a matrix multiplication. Therefore, a

diagonal representation for Green's functions is not assumed.

Arbitrary non- equilibrium: No assumptions about slowly varying disturbances, small deviations from equilibrium, or quasi-particle approximation are built in, the Ansatz is formally quite general.

The GKBA particle correlation function perfectly fits into the formal NGF scheme. It was constructed in this manner in order to overcome the limitations of the KBA. When inserted into the machinery of deriving quantum transport equations from the NGF, it leads, as described already in the Introduction, to the GME, rather than to the BE like quantum kinetic equations. For these purposes, it has been amply used. All this is the subject matter of Paper III.

The GKBA also has an important meaning, independent of and going beyond the restricted context of transport equations. Namely, it offers an alternative path to the Reconstruction Problem, as will be outlined here.

Comparing (67) with (62), we may state that the *GKBA is the utmost extension of the Fluctuation Dissipation formula to non-equilibrium*. The related interpretation resembles that of the KBA: starting from the reduced information in ρ and the propagators, the GKBA permits to reconstruct the whole particle correlation function as their product.

There is a basic difference, however, which distinguishes the GKBA from the KBA. Namely, while both Ansatzes are but approximate constructions, expression (67) can, in addition, serve as a starting approximation for a process leading to an exact reconstruction of $G^<$.

This assertion is valid in this simple form, and can be demonstrated, for the case of uncorrelated initial conditions. From Eq. (40), there follows a couple of appropriate Dyson type equations for $G^<$, reported in [17] and discovered independently by Vinogradov [18]; see also [8,9].

To illustrate their derivation and interpretation, we start by observing that the GKBA expression (67) for $G^<$ consists of two distinct parts, one for $t_1>t_2$, the other one for $t_2>t_1$ and The exact $G^<$ is split in the corresponding way:

$$G^<(t_1,t_2) = G^<_{\rm R}(t_1,t_2) - G^<_{\rm A}(t_1,t_2), \tag{68}$$

$$G^<_{\rm R}(t_1,t_2) = \theta(t_1-t_2)G^<(t_1,t_2), \tag{69}$$

$$G^<_{\rm A}(t_1,t_2) = -\theta(t_2-t_1)G^<(t_1,t_2) = [G^<_{\rm R}(t_2,t_1)]^\dagger\ . \tag{70}$$

It is convenient to calculate

$$\begin{aligned}
&\{G^{\rm R}\}^{-1}G^<_R|_{t_1,t_2}\\
&\quad = (G_0^{-1}-\Sigma^{\rm R})G^<_R|_{t_1,t_2}\\
&\quad = \delta(t_1-t_2)\rho(t_2)\\
&\qquad + \theta(t_1-t_2)(\{G^{\rm R}\}^{-1}G^<\\
&\qquad + \Sigma^{\rm R}G^< - \Sigma^{\rm R}G^<_{\rm R})|_{t_1,t_2}\\
&\quad = \delta(t_1-t_2)\rho(t_2)\\
&\qquad + \theta(t_1-t_2)(\Sigma^<G^{\rm A} + \Sigma^{\rm R}G^<_{\rm A})|_{t_1,t_2}.
\end{aligned} \tag{71}$$

where Eqs. (33), (34) and (37) were employed. Multiplication by G^R from the left yields the first equation for $G^<_{\rm R}$, that is for $G^<$ valid in the $t_1>t_2>t_0$ wedge:

$$\begin{aligned}
G^<(t_1,t_2) = &-G^{\rm R}(t_1,t_2)\rho(t_2)\\
&+\int_{t_2}^{t_1}{\rm d}\bar{\bar{t}}\int_{t_0}^{t_2}d\bar{t}G^{\rm R}(t_1,\bar{\bar{t}})\Sigma^<(\bar{\bar{t}},\bar{t})G^{\rm A}(\bar{t},t_2)\\
&+\int_{t_2}^{t_1}{\rm d}\bar{\bar{t}}\int_{t_0}^{t_2}d\bar{t}G^{\rm R}(t_1,\bar{\bar{t}})\Sigma^{\rm R}(\bar{\bar{t}},\bar{t})G^<(\bar{t},t_2).
\end{aligned} \tag{72}$$

In the complementary time region $t_0<t_1<t_2$, the equation for $G^< = G^<_{\rm A}$ is quite similar. It can be obtained as a conjugate to (72), as it holds that $G^<(t_1,t_2) = -[G^<(t_2,t_1)]^\dagger$. It starts as

$$\begin{aligned}
G^<(t_1,t_2) = &\rho(t_1)G^{\rm A}(t_1,t_2)\\
&+\cdots.
\end{aligned} \tag{73}$$

The absolute terms of equation pair (72) and (73) together form the GKBA expression (67). The two integral terms contain the unknown $G^<$: the second one explicitly, and the first one through the functional dependence $\Sigma^< = \Sigma^<[G^<]$.

We may conclude that by solving Eqs. (72) and (73), the double-time correlation function $G^<(t_1,t_2\neq t_1)$ is generated from the knowledge of its time-diagonal part, the one-particle single-time density $\rho(t)\propto G^<(t,t)$, and of the propagators also taken as known. This result in itself has the

importance of the *exact non-equilibrium counterpart to the Fluctuation Dissipation Theorem*. Furthermore, it represents the first, and the most important step to the NGF Reconstruction Theorem.

Eqs. (72) and (73) can also be used as they stand in two alternative ways. On the one hand, they are perfectly suited for a direct numerical solution aiming at $G^<$ connected with a particular physical situation. So far, no computation of $G^<$ along these specific lines has been reported. On the other hand, the reconstruction equations (72) and (73) can serve the important purpose of generating gradually improving Ansatzes by formal iteration. The use of such an improved *renormalized GKBA Ansatz* would be to introduce it into the interaction terms of the precursor transport Eq.(56) in order to convert it to a closed GME for ρ. This is a well-defined route to a family of presumably more and more precise GME.

8.4. The NGF Reconstruction Theorem

To clarify the meaning of the Theorem, first we have to see, what is the necessary input for obtaining $G^<$. (i) At equal times, Eqs. (72) and (73) turn to tautology. The "time diagonal" ρ is one of the input quantities and has to be known beforehand. (This trivially includes the un-correlated initial condition (39).) (ii) We assumed throughout that the propagators and their self-energies are somehow known. This is not trivial beyond equilibrium and, in fact, the propagators have to be found in another process, too.

The NGF Reconstruction Theorem is obtained by choosing an appropriate order of steps in solving the full NGF problem. At the hub of the whole process stands the *single-particle distribution* ρ. It is obtained by solving the exact precursor of the GME, the so-called *GKB Equation*, which is obtained by joining Eqs. (44) and (45)

$$\frac{\partial\rho}{\partial t} + \mathrm{i}[H_0,\rho]_- = -\mathrm{i}[-G^{\mathrm{R}}\Sigma^< + \Sigma^< G^{\mathrm{A}} + \Sigma^{\mathrm{R}}G^< - G^<\Sigma^{\mathrm{A}}]_{t_1=t=t_2}. \quad (74)$$

To convert the GKBE to a closed transport equation for ρ, we have to specify the *physical approximation for the self-energies* in the form $\boldsymbol{\Sigma} = \boldsymbol{\Sigma}[\mathrm{G}]$, that is, more explicitly,

$$\Sigma^{\mathrm{R,A}} = \Sigma^{\mathrm{R,A}}[G^{\mathrm{R,A}}, G^<], \quad \Sigma^< = \Sigma^<[G^{\mathrm{R,A}}, G^<]. \quad (75)$$

Next, the pair of *reconstruction equations* (72), (73) is used to express $G^<$ in the functional form

$$G^< = G^<[\rho, G^{\mathrm{R,A}}]\,. \quad (76)$$

Finally, the *Dyson equations for propagators* (see (36))

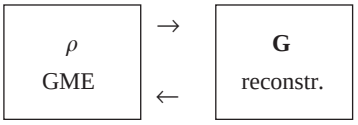
$$G^{\mathrm{R}} = G_0^{\mathrm{R}} + G_0^{\mathrm{R}}\Sigma^{\mathrm{R}}G^{\mathrm{R}},$$
$$G^{\mathrm{A}} = G_0^{\mathrm{A}} + G_0^{\mathrm{A}}\Sigma^{\mathrm{A}}G^{\mathrm{A}}. \quad (77)$$

link the problem with the non-interacting particles and incorporate the effective external field as a boundary condition.

The full NGF set G^{R}, $G^<$, G^{A} is obtained by a simultaneous solution of Eqs. (74)–(77).

The NGF Reconstruction Theorem

The contents of the Reconstruction Theorem appears to be such that the determination of the full NGF set G^{R}, $G^<$, G^{A} can be structured to a dual process. In one stream, the single-particle distribution ρ is obtained from a closed GME type transport equation. In the other stream, the NGF is reconstructed from known ρ. The two streams are mutually coupled:



(78)

This prompts a simultaneous treatment of the whole task, which is only possible by a solution in successive steps.

These steps may progress incrementally in time. Starting from the initial $\rho(t_0) = \rho_{\mathrm{init}}$, see Eq. (39), all quantities are obtained step by step rimming the already covered time region $[t_0, t] \otimes [t_0, t]$ by a strip having a width of the time increment Δt. It is easy to verify that all equations involved have the causal structure appropriate for this protocol. The experience with similar tasks suggests that this will be a practicable technique [62].

An alternative method would be an iteration of the equations with respect to some expansion parameters. While less promising for computations, the iteration scheme has a more basic context. Namely, it is important to select and interpret the iteration procedure. There are two standpoints here, and their relationship is not entirely clear.

I. Interaction strength as a small parameter

Clearly, for non-interacting particles, the self-energies and Eqs. (72) and (73) demonstrate that the GKBA is exact in this limiting case. Thus, the iteration of the equations might be interpreted as a perturbation expansion depending on the particle interaction strength. This point of view has been expressed several times, and it is not unjustified. If the whole reconstruction reduced just to this, it would be brought rather close to the direct methods of deriving the GME, which are often based on some notion of a weak influence of the particle interactions.

II. Collision duration time as a small parameter

When comparing the original Eq. (42) for $G^<$ with (72) and (73), an important characteristic feature of the latter is conspicuous: the off-diagonal integration regions of the double integrals:

$$t_0 \leqslant \bar{t} \leqslant t_2 \leqslant \bar{\bar{t}} \leqslant t_1.$$

Both integration variables converge in the self-energies $\Sigma^<(\bar{\bar{t}}, \bar{t})$, $\Sigma^{\mathrm{R}}(\bar{\bar{t}}, \bar{t})$. Only the off-diagonal blocks of the self-energies joining the past and the future are contributing. The small parameter determining the importance of the corrections to the GKBA in, say, Eq. (72) is, loosely speaking, the width of the strip around the time diagonal, in which the values of self-energies are significant. The respective characteristic times, τ_Q for Σ^{R} and τ_c for $\Sigma^<$, may be different, but both should be "small". On the physical side, we see that, rather than the strength of the interactions, it is their inner dynamics which is decisive for the iteration procedure. This dynamics is reflected in the memory for build-up processes induced in the system during a non-equilibrium evolution. In fact, the two characteristic times are best defined in an operational way from Eqs. (72) and (73). Whether they are small or not, that depends on the process in question and the related characteristic times. Thus, there is no absolute criterion for validity of the GKBA or its iterates.

It should be pointed out that with this second interpretation of the Ansatz scheme, the whole path to the quantum transport equations outlined in this section has practically the same physical background as the direct methods based on the superprojection techniques. There may be a practical difference, however, in the relative ease of actual construction of the quantum transport equation in the NGF method, where the elements used are all single-particle, although double-time, characteristics and the whole scheme is consistently renormalized at each level of approximation.

Another comparison relates to the TDDFT. The NGF Reconstruction Theorem concerns the stage of reconstruction up from the one-particle density matrix. The Runge Gross Theorem is more specific in showing that the necessary reduced quantity is, in fact, the local particle density, that means only the space diagonal of the density matrix. This is correct for a local external field; in our treatment, no specific property of the external potential was employed, in fact. For the more general situation of a possible non-local field, the reduction to the full ρ is to be expected. The other difference concerns the proof of the Theorem. In the NGF case, it is constructive, so that the proof also contains the algorithmic basis for an actual reconstruction. Otherwise, the relationship of both approaches remains close, and hybrids, or offsprings of both may be promising in the future.

9. Conclusions

This paper served several purposes:

(1) to summarize the present views on construction of the quantum transport equations based on the NGF approach;
(2) to characterize the position of the NGF among other theoretical techniques for non-equilibrium systems;

(3) to analyze the physical and formal context of the so-called Ansatz decouplings;
(4) to explore the status of the so-called Reconstruction Theorems, which try to show that an exact description of a non-equilibrium system in terms of one-particle quantities is possible. Such ideas are at the core of the density functional theory. We presented a comparison between the TDDFT and the properly renormalized NGF formalism. There is a close relationship between both formalisms and they may tend to merge in the future.

The general outcome of our analysis is favorable. The discussed approaches and their results have been rather successful and form a basis for future work aiming at a description of complex processes far from equilibrium, typically involving coherent short time dynamics in response to fast disturbing fields, which is followed by early relaxation and equilibration processes evolving on the intermediate time scale.

The two attached Papers II and III are devoted to a more detailed treatment of the different time scales for quantum transport processes and to a lesser extent to the bridging periods between them.

Acknowledgements

This research was partially supported by the Grant Agencies of the Czech Republic and of the Academy of Sciences within the grant projects 202/04/0585 and A1010404, respectively. The research was carried out by V.S. within the Institutional Research Plan AV0Z10100521 and by A.K within the Institutional Research Plan AVOZ10100520, both financed by the Academy of Sciences of the Czech Republic. The work of B.V. is a part of the research programs MSM 0021620834 and MSM 0021620845 financed by the Ministry of Education of the Czech Republic.

Long years of collaboration with Pavel Lipavsky, who contributed essentially to much of the material and ideas covered, are gratefully acknowledged. We are also grateful to Klaus Morawetz for friendly scientific collaboration and many inspiring conversations. We also thank A. MacKinnon, M.Bonitz, R. Zimmermann, D. Kremp, H. Haug, A.–P. Jauho, and C.Caroli for illuminating discussions.

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